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13. ABSTRACT *(Maximum 200 words)*

This project aimed first at obtaining a better understanding of numerical methods for hyperbolic conservation laws. Several significant advances were obtained. In particular, the interplay between the size, uniformity and topology of numerical grids and the accuracy of numerical solutions based on those grids has been uncovered. This type of results in unique for problems with low regularity. Those a priori estimates have led to the first explanation of supraconvergence for conservation laws. The possibility of using earlier results, a posteriori estimates, for the design of adaptive methods with full mathematical backing was also investigated.

In a second part, numerical methods for related problems were considered. For systems of Hamilton-Jacobi equations, the notion of viscosity solution cannot be applied. In spite of this, competitive numerical methods were constructed and successfully used. The flow of granular materials, a highly important but ill-understood problem, was also considered. Those problems have several nonstandard features. Computational results based on the first implementation, in that field, of higher order numerical (Discontinuous Galerkin) methods were obtained. A code is currently being tested by engineers in an industrial setting.

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1. LIST OF FIGURES:

2. STATEMENT OF THE PROBLEMS STUDIED:

The various goals of the project were clearly stated in the main proposal. Seven of them, widely different in length and difficulties were explicitly listed; they were

(1) derivation of optimal error estimates for multidimensional monotone schemes for conservation laws,
(2) generalization to schemes that do not possess splitting fluxes,
(3) generalization to higher order methods,
(4) study of the possibility, or lack thereof, of generalization to systems of conservation laws,
(5) derivation of general a posteriori estimates,
(6) design and implementation of mathematically sound adaptive strategies for hyperbolic problems,
(7) applications to granular flows and other problems (in particular Hamilton-Jacobi equations, even though those were not explicitly mentioned in the proposal).

3. SUMMARY OF THE MOST IMPORTANT RESULTS:

Significant advances were obtained for most, but not all of the above problems. People who collaborated with the PI on questions covered by the project at one point or another, but were not directly supported by it, include Profs. G. Amiez, (U. of Franche-Comté, France), V. Alexiades (U. of Tennessee), B. Cockburn (U. of Minnesota), D. Schaeffer (Duke University) and M. Shearer (North Carolina State University), as well as K.S. Lowder (former graduate student, Gremaud adviser, U.S. Airforce Academy), N.R. Ide (former graduate student, Gremaud adviser, Lincoln Lab, MIT), J.V. Matthews (current Ph.D. student, Gremaud adviser), and W. Turner (former graduate student, Gremaud adviser, NCSU). We have also worked in consultation with Engineers at Jenike & Johanson, Inc., Westford, MA., and in particular T.A. Royal, Vice President, to develop efficient and robust solvers for various types of problems related to granular flows.

The accomplishments corresponding to the above categories are now reviewed. In a first part, the work pertaining to error estimates for conservation laws is discussed (parts (1) through (6)). A second part deals with the advances related to both Hamilton-Jacobi equations and granular materials. Finally, some remarks on ongoing and future work are offered.

Error estimates for numerical conservation laws (parts (1)-(6)).

The goal was here to estimate the error between the weak entropy solution v to a generic scalar conservation law

$$\partial_t v + \nabla \cdot f(v) = 0,$$
$$v(\cdot, 0) = v_0.$$

and a numerical solution u constructed from as general a method as possible. Several aspects of those types of hyperbolic problems makes this a challenging task, namely the presence of shocks and the existence of many weak solutions, among which only the entropy solution is believed to have a physical meaning.

Our main contribution is the derivation of a priori estimates, i.e., estimates written only in terms of the exact solution. Those estimates are of the form

$$e(T) \leq \Phi(v, T),$$

where $e(t)$ denotes the L^1-error at time t. Our results are the first and only rigorous error estimates of this type for nonlinear conservation laws. *All* the other results we are aware of are of the form

$$e(T) \leq \Psi(v, u, T),$$

i.e., they also involve the approximate solution u. If Ψ does not involve v but only u, the latter estimate is referred to as an a posteriori error estimate.

At the beginning of this proposal, virtually every error estimate was based on an original approach by Kuznetsov (1976). In a joint work with B. Cockburn (1996) that took place slightly before the start of the present project, we identified Kuztnetsov's point of view as an a posteriori approach. This was then applied to the derivation of a posteriori error estimates for both shock capturing streamline diffusion methods and shock capturing discontinuous Galerkin methods. A posteriori estimates are very useful for practical computations if they are properly used as part of an adaptive strategy. Part of the present project, see part (6) above, dealt with those very issues. Essentially, our a posteriori estimates are as follows

$$e(T) \leq e(0) + C\| \partial_t \Pi_h(u) + \nabla \cdot f(t, x, \Pi_h(u)) \|_{L^1(0,T,L^1)}$$

where C is a numerical constant, Π_h an interpolation operator into a finite dimensional space of continuous, and thus $\partial_t \Pi_h(u) + \nabla \cdot f(t, x, \Pi_h(u))$ is the residual. The feasibility of using such a result as the basis for an adaptive strategy was studied for instance in K. Lowder, *Mesh Optimization for Conservation Laws*, Master's Project, Dept. of Mathematics, NCSU, Gremaud Adviser (1996). The point of view taken there was to obtain a "close to optimal" mesh at each time, based on the error estimate. The results were mixed. In the simplest cases tried, the grids were successfully adapted to the features of the solution. However, first, it came at considerable computational cost. Second, for more involved cases, the construction of the residual, for instance the *choice* of a proper interpolation operator Π_h in the above expression, played a crucial role. We were not able to find a general way of constructing such a operator that would work for "all" cases. Here again, having to deal with possibly discontinuous solutions is a significant complicating factor. The algorithms obtained were not competitive with most of the common heuristic methods in this field, as far as adaptivity is concerned.

A natural next step consisted then in improving our understanding of the influence of the grid on the accuracy of the numerical solution. Indeed, an adaptive strategy is likely to change the *size*, the *uniformity* and the *topology* of the grid. The best way of studying those effects is through a priori error estimates. This project has led to very significant improvements in that respect.

It has been known from quite some time that if the numerical fluxes do not properly take into account the irregularities of the grid, a loss of consistency occurs. This can be shown on very simple examples, for which the truncation error does not go to zero, see e.g. [8] below. The fact is, that in most practical codes, numerical fluxes *are not* modified to take into account local mesh variations. Yet, those codes perform quite well, and not only converge to the correct solution, but may in fact do so without loss in the order of convergence, this, in spite of the loss of consistency. This *supraconvergence* phenomenon remained unexplained for nonlinear conservation laws until the publication of [8], and [7] after that. The approach is based on a modification of Kuznetsov's original approximation theory. The point of view taken is essentially the dual of Kuznetsov's, and does lead to a sound a priori theory. This was applied in [8] to monotone schemes on nonuniform Cartesian grids, and in [8], to monotone on general multidimensional grids. An interesting point is related to the importance of the topology of the grid. It is known (Sanders, 1983) that for monotone schemes on *Cartesian* grids, uniform or not, the total variation of the numerical solution does not increase in time. This is not true for *non-Cartesian* grids, even uniform ones. Indeed, in [7], a simple example is presented on a uniform grid consisting of equilateral triangles, and hence non-Cartesian, for which even the Lax-Friedrichs scheme presents an increase in total variation. This shows that the case of non-Cartesian grids is intrinsically, not just technically, more complex. The estimates in [7] are given in terms of quantities measuring, for general multidimensional grids, the departure from Cartesianity and uniformity. This work is the first rigorous explanation of the abovementioned supraconvergence phenomenon. In essence, what happens is that the possible lack of consistency of the numerical methods is in fact compensated providing two fundamental properties are satisfied: first, the methods are *conservative*, second, the numerical fluxes are *consistent* (not to be confused with the consistency of the entire method).

The above approach can *in principle* be applied to higher order methods. It is in fact the only theoretical approach we know for which this statement can be made in a reasonably general sense. However, the shear technical complexity is enormous. This point remains under study. Another aspect was the possibility, or lack thereof, of a generalization of the above results to *systems* of hyperbolic conservation laws. Here, the difficulties are not technical, but conceptual, since in fact the whole notion of entropy solution becomes problematic for systems. The Numerical Analysis of such problems remains essentially an open problem. It would appear that what is needed is not some kind of incremental improvement, built on the available theory, but a complete breakthrough. There have been, however, progresses made during the period of this project related to the understanding of systems of first order nonlinear Partial Differential Equations, see in particular the work below in systems of Hamilton-Jacobi equations.

Applications: Hamilton-Jacobi equations and granular materials.

As mentioned above, the case of *systems* of conservation laws is still largely an open problem. Recent results have however been obtained for Hamilton-Jacobi equations, both in the scalar and vectorial cases (Dacorogna-Marcellini, 1996). Essentially, those results apply to cases for which the usual viscosity approach is either ill-suited or not applicable. An important application is solid-solid phase transition problems, which are usually expressed as multi-well potential problems. Those can be recast as systems of Hamilton-Jacobi equations, an entirely new approach.

We have proposed and tested a numerical approach for the calculation of solutions to Hamilton-Jacobi equations under a viscoelasticity/capillarity criterion. The (very weak) notion of "satisfying the boundary conditions in the viscous sense" as well as the nonexistence of the very notion of viscosity solution in the vectorial case prevented us from using the classical viscosity criterion. The challenge was to construct methods that would convergence to a properly selected solution in the scalar and in the vectorial case. The idea of the methods consists in discretizing the original PDEs by finite difference formulas of sufficiently high order as to guarantee the model equations to be identical to the PDEs. Anything short of that would lead, and indeed did lead, to an effective modification of the selection criterion. The approach is used in conjunction with a pseudotime integrator of the BDF type. Before this work, almost all the results dealing with the use of the above selection criterion were for scalar equations in the 1d case. We have not only treated multidimensional scalar problems, but also multidimensional *vectorial* ones. We are not aware of other numerical results about vectorial Hamilton-Jacobi equations. Practically speaking, the advantage of the method is as follows. For typical solid-solid phase change problems, the traditional approach is to construct an energy functional (always nonconvex, unless the problem is trivial), discretize the corresponding variational problem, and then solve somehow the corresponding discrete strongly nonconvex minimization problem. As is well known, nonconvex minimization is hard, and the methods likely to be used, at least in the case of solid-solid phase change problems, are likely to be ad hoc, and void of any physical justification. The aim here was to bypass the minimization problem by solving to steady state a physically meaningful problem (time dependent Hamilton-Jacobi system). The feasibility of the approach was illustrated in [3].

The last part of the project involves the study of an important type of application: the study of the flow of granular materials. In the general subject of industrial flows, it can be argued that granular flows are as important as fluid/gas flows (see agriculture, chemical, construction and pharmaceutical industries to name but a few). In spite of this, those problems have received very little attention. Part of this project deals with those problems (see part 4, project abstract, p. C-1.).

One of the first and main problems one encounters when dealing with granular materials is to obtain a proper mathematical model. Several models exist, that appear to capture well some, but in general not all, aspects of the phenomena under consideration. Our approach is twofold. First, we aim at obtaining, through careful Analysis and Numerical Analysis of existing models, efficient and reliable computational tools that will allow for meaningful investigations the models themselves, through comparisons with experiments for instance. Second, and at a less fundamental level, having such computational tools represents a breakthrough in this field, and open new opportunities in terms of numerical simulations in industrial settings.

So far, our study has been restricted to established hopper flows. This constitutes in our view a first, meaningful, step toward the study of more general problems, as discussed below. Equations governing the *time dependent* flow of granular material under gravity can be derived and analyzed. However, those are found to be linearly illposed in most cases of practical interest. To our knowledge, the situation is not fully understood, mathematically or otherwise. In practice, strongly time-dependent problems are usually observed in conjunction with *funnel flows*, i.e., flows for which the motion is essentially restricted to the central part of the silo. Our study has dealt, so far, exclusively with *mass flows*, i.e., flows for which all the material is mobilized. In this context, established, steady state flows can be observed.

In a nutshell, our contributions have been

(1) construction and implementation of cellular automaton model for hopper flows,
(2) investigation of the properties and stability of radial stress fields for various plasticity models,
(3) investigation of extensions of the notion of radial solutions, and their possible use as design tools for flow corrective inserts,
(4) first implementation of a highly accurate method (Discontinuous Galerkin method) for the computation of hopper flows,
(5) computation of "switch stresses" due to changes of the hopper's wall angle.

We now proceed to describe in more details the above points.

Cellular automaton. A simple cellular automaton model was designed. The idea is essentially to work with discrete particles, that can only be in "states" taking values in some discrete spaces. In spite of its simplicity, this type of models allowed us to predict structure formations reminiscent of the density waves observed experimentally with some hopper flows, see [9] for details. However, the approach also suffers from serious drawbacks. In particular, by its very nature, all the information available from such simulations is at the particle level. It is not always obvious and/or convenient to translate this into quantities that can be experimentally measured. Further, an obvious bottleneck is the number of particles that can be treated. The continuum approach, that we have adopted since then, has none of those disadvantages.

Radial solutions. In some cases of industrial importance, such as axisymmetric containers (silos), similarity solutions (radial solutions) can be constructed. Most of the existing work in this field is in fact based the use of those solutions. This is especially true of the Engineering literature. In [6], those solutions were constructed for two plasticity models, namely for Mohr-Coulomb and von Mises yield conditions. Comparisons of the stress and velocity fields for the two models gave a better picture of their respective properties. Further, in the simplest of the two cases (Mohr-Coulomb), a numerical stability study was performed. Thanks to the use of a highly accurate method (pseudospectral Chebyshev collocation method), a fairly complete picture of the influence of the material parameters, such as internal friction and wall friction, on the stability was uncovered.

Extension of the notion of radial solutions. The notion of radial solution has several obvious shortcomings. Prime among those is the fact that it only exists in radially symmetric domains. As an attempt to alleviate this limitation, we have studied the possibility of considering the radial solution as the first term in an expansion of the following type

$$T(r,\theta) = rT^0(\theta) + r^2T^1(\theta) + \dots$$
$$v(r,\theta) = \frac{1}{r}v^0(\theta) + v^1(\theta) + \dots .$$

where T and v stand for generic stress and velocity components respectively. The zero-th order terms correspond to the radial solution. This approach was explored in [6] were it was applied to non radially symmetric domains, and specifically to the determination of flow corrective inserts. Although the approach was successful, it also brought to light several limitations of even this type of extensions of the radial field. More precisely, it turns out that in many cases of practical interest, the above expansion converges too slowly to be competitive with the resolution of the full system of equations, which we discuss now.

Numerical resolution of the full system of equations. The full system of equations correspond to the laws of conservation of mass and momentum. In the simplest case, i.e., Mohr-Coulomb materials, the stress equations decouple from the velocity equations (the later still depend on the stresses). The stress equations correspond then to a pair of hyperbolic conservation laws with source terms and nonlinear boundary conditions. To date, most attempts toward the numerical simulation of the corresponding solutions have been based on a judicious change of variables. Indeed, the yield condition corresponds to an algebraic constraint which can be "solved". In other words, when using the so-called Sokolowskii variables the constraint is automatically satisfied. Numerical methods can be then used to solve the reformulated system, for instance in terms in the Riemann invariants, which was our first approach.

However, and in spite of its popularity, the use of those Sokolowskii comes at a heavy price: the conservative form of the equations is lost, and thus, so is the ability to analyze and/or compute shocks. One has to conclude that the equations should in fact preferably be solved in the original variables, even at the price of having to deal with a corresponding complicated hyperbolic flux term (no a priori bounds on the wave speeds). Further, the discretization of the equations in conservation form has several advantages from a purely numerical point of view. We have implemented an algorithm corresponding to a formally globally third order Discontinuous Galerkin method for the resolution of three dimensional axisymmetric hopper flows involving Coulomb materials. The approach has been extremely successful.

Computation of switch stresses. As a way of illustration, we include hereafter calculations corresponding to the influence on the stress field of abrupt changes in the wall angle. The geometrical situation is as follows

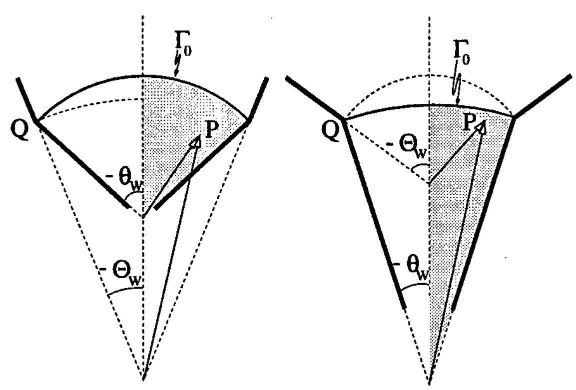

FIGURE 1. *Geometrical situation; left: transition to a flatter wall angle, right: transition to a steeper wall angle. The radial stress is used to generate an initial condition on the curve Γ_0. The domains of calculation are shaded.*

In the case of a transition from a steeper to a flatter hopper, the following type of structure is observed

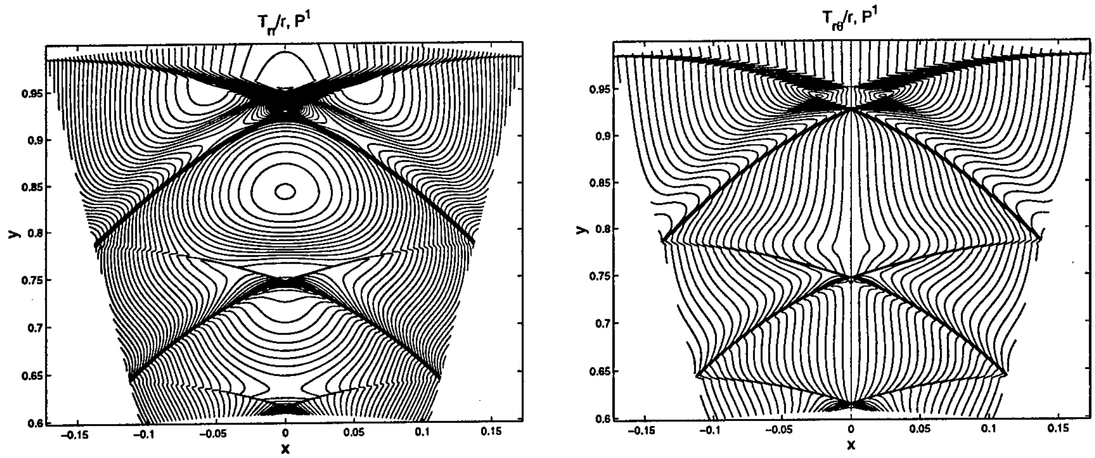

FIGURE 2. *Structure of the stress field induced by a transition from an opening angle of* 10^o *to one of* 15^o. *The actual geometry of the hopper is represented.*

If instead, the wall goes from flatter to steeper, the stress field takes the following form

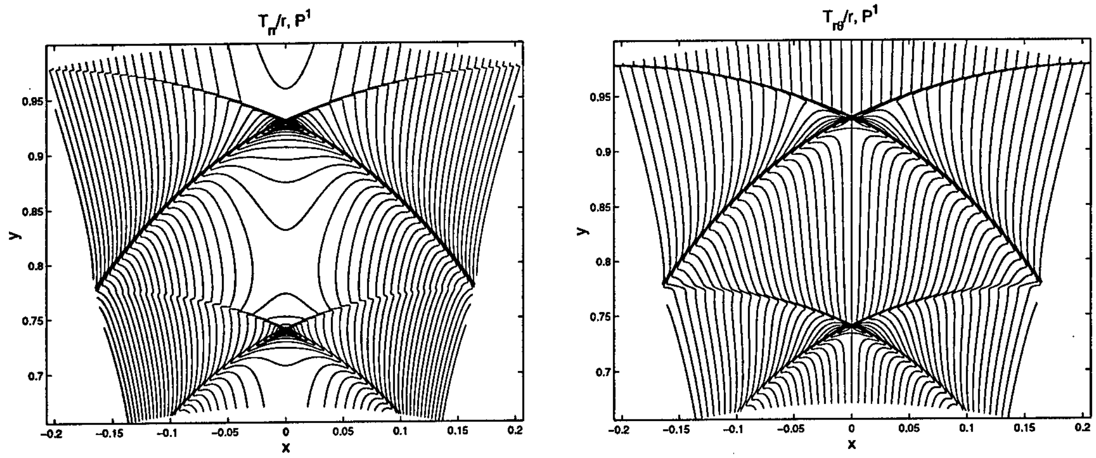

FIGURE 3. *Structure of the stress field induced by a transition from an opening angle of* 10^o *to one of* 12^o. *The actual geometry of the hopper is represented.*

We are not aware of other successful calculations of this type of effects. The corresponding equations are quite delicate to handle numerically because of the interplay between the source terms and the nonlinear boundary conditions. Further, some assumptions related to the structure of the above waves can be found in the literature. It has for instance been conjectured that a transition to a flatter hopper, see Figure 2, would induce shocks, while a transition to a steeper one, see Figure 3, would corresponding to rarefaction types of waves. Those claims are typically based on unsubstantiated arguments, for instance on a radial solution analysis. This cannot make sense here because of the lack of symmetry of the full domain, see Figure 1. Figures 2 and 3 suggest that the situation is in fact more complicated. A full analysis of those results is under way. Experimental comparisons can be done for instance based on the values of the normal stress on the wall predicted by the numerics. This type of comparison is also under way, specifically for cereal types of grains in steal hoppers for instance.

Ongoing and future work about granular materials. We list hereafter ongoing and future work, starting from tasks that are well under way or expected to present no major difficulties, to more involved problems.

(1) **Resolution of the velocity equations.** Within our current model, the velocity equations consist in an additional pair of hyperbolic conservation laws coupled to the stresses, to which the same numerical approach (essentially the same Discontinuous Galerkin code) can be applied. One of the challenges lies here in determining how the velocity "information travels". We expect a careful numerical study to bring an answer to this type of questions, that are for now open.

(2) **Computation of flows around obstacles.** Assuming the flow is still consistent with the assumptions of the models, this computation can be done without further difficulties.

(3) **Inclusion in the models of interstitial fluids.** When dealing for instance with fine powders or soils (clay, etc...), the presence of interstitial fluid cannot be neglected. The models have then to be revised to include the corresponding effects. So far, our work in this direction has been limited to the study of the consolidation of fine powders. *Further, many problems of prime interest to the Army such as mine detection or soil vehicle interactions are by nature quite close to both the computation of flows around obstacles and the present question of interstitial flows.* Plowing is another example. Preliminary contacts have been taken with Drs. J.F. Peters and D.A. Horner at the U.S. Army Engineer Waterways Experiment Station in Vicksburg, MS (visit to WES in Oct. 98), to explore this further.

(4) **Determination of more general switch stresses.** We cannot treat, in the present context, the case of the transition from a *vertical* pipe to a conical hopper. The reason is that in the vertical pipe, the granular material is thought to be in an *active* state, as opposed to a *passive* state as in any conical hopper. This change corresponds mathematically, in our current setting, to a discontinuity in the hyperbolic flux function itself. The model as it stands does not allow for the prediction of where the transition between active and passive kind of flows takes place.

(5) **Long term objectives.** Among the long term objectives, we include the possibility of solving the above problems for a wider range of constitutive laws, such as for instance critical state soil mechanics, the possibility of computing and analyzing rigid-plastic free boundaries, as well as the treatment of fully time dependent problems.

4. TECHNOLOGY TRANSFER:

We will pursue our collaboration with Jenike & Johanson, Inc. After our recent visit there, the focus will be on the efficient resolution of the full problem for granular flows (as described above). One of the common goals is the construction of numerical solvers that work in nontrivial geometries (hopper with insert, for instance), and for a wide variety of materials. Additional contacts have already been scheduled. Further, our numerical code for the resolution of powder consolidation problems in currently (Summer 99) being tested by the engineers at Jenike & Johanson. This code, which uses a Differential Algebraic Equation approach to the problem of determining stresses, air pressure and height of a column of powder in an axisymmetric geometry is of immediate practical use.

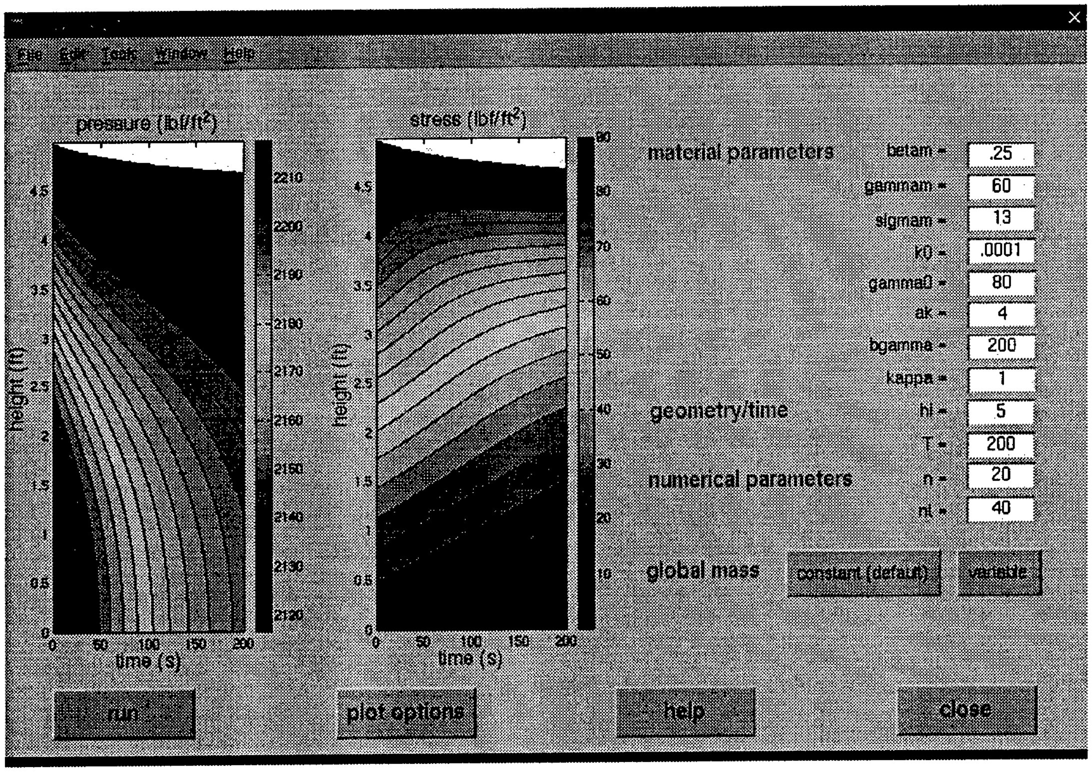

FIGURE 4. *Graphic user interface, GUI, for the powder consolidation problem, being tested at Jenike and Johanson, Inc.*

We also intent to explore further the possibility of collaborating with the researchers at the U.S. Army Engineer Waterways Experiment Station in Vicksburg, MS, especially in terms of the possible use the present continuum approach to "plowing type problems".

5. LIST OF MANUSCRIPTS SUBMITTED OR PUBLISHED UNDER ARO SPONSORSHIP DURING THIS PERIOD, INCLUDING JOURNAL REFERENCES:

(1) with D. Schaeffer and M. Shearer, *Numerical determination of flow corrective inserts for granular materials in conical hoppers*, NCSU CRSC-TR98-34 (Oct. 98) Technical report, to be published in *Int. J. Nonlinear Mech.*

(2) with J.V. Matthews, *Simulation of Gravity Flow of Granular Materials in Silos*, Proceedings of the International Symposium on Discontinuous Galerkin Methods, Newport, RI (May 1999), B. Cockburn, C.W. Shu, G. Karniadakis Eds., (10 pages), Springer Verlag, to be published.

(3) with N. R. Ide, *Computation of Nonclassical Solutions to Hamilton-Jacobi Problems*, (20 pages), to be published in *SIAM J. Sci. Comput.*

(4) with B. Cockburn and Xiangrong Yang, *New Results for Numerical Conservation Laws*, Proceedings of the Interdisciplinary Congress on Free Boundary Problems, Theory and Applications, Herakleion (Crete), Grece, June 1997, Longman, to be published (11 pages).

(5) with B. Cockburn and Xiangrong Yang, *A priori error estimates for nonlinear conservation laws*, Proceedings of the Seventh International Conference on Hyperbolic Problems, ETH Zurich, Switzerland, Feb. 1998, to be published.

(6) with J.V. Matthews and M. Shearer, *Similarity solutions for hopper flows*, NCSU CRSC-TR98-47 (Dec. 98), to be published in the Proceedings of the SIAM/AMS Conference on Nonlinear PDEs, Dynamics and Continuum Physics, J. Bona, K. Saxton, R. Saxton, Eds., AMS Contemporary Mathematics Series.

(7) with B. Cockburn and Xiangrong Yang, *A Priori Error Estimates for Numerical Methods for Scalar Conservation Laws. Part III: Multidimensional Flux-Splitting Monotone Schemes on Non-Cartesian Grids*, *SIAM J. Numer. Anal.*, 35 (1998), p.1775–1803.

(8) with B. Cockburn, A Priori Error Estimates for Numerical Methods for Scalar Conservation Laws. Part II: Flux-Splitting Monotone Schemes on Irregular Cartesian Grids, *Math. Comp*, 66 (1997), p.547–572.

(9) Numerical Simulation of Pattern Formation in Grain Flows, *Appl. Math. Comp.*, 84 (1997), p.145–162.

(10) V. Alexiades and G. Amiez), Super-Time-Stepping Acceleration of Explicit Schemes, *Com. Num. Meth. Eng*, 12 (1996), p.31–42.

(11) with B. Cockburn, A Priori Error Estimates for Numerical Methods for Scalar Conservation Laws. Part I: The General Approach, *Math. Comp.*, 65 (1996), p.533–573.

(12) with B. Cockburn, An a priori-a posteriori Approach to Numerical Conservation Laws, Proceedings of the International Congress on Industrial and Applied Mathematics, ICIAM 95, Hamburg, Germany, *Z. Ang. Math. Mech., 76 S1 (1996), p.379–380.*

6. SCIENTIFIC PERSONNEL SUPPORTED BY THIS PROJECT: P.A. Gremaud, PI.